Carbonic acid, 2,2,2-trichloroethyl cyclohexylmethyl ester

Inchi: InChI=1S/C10H15Cl3O3/c11-10(12,13)7-16-9(14)15-6-8-4-2-1-3-5-8/h8H,1-7H2

InchiKey: XMERHXQQEIBUTR-UHFFFAOYSA-N

Formula: C10H15Cl3O3

SMILES: O=C(OCC1CCCCC1)OCC(Cl)(Cl)Cl

Mol. weight [g/mol]: 289.58

Physical Properties

Property code	Value	Unit	Source
gf	-314.10	kJ/mol	Joback Method
hf	-628.40	kJ/mol	Joback Method
hfus	22.64	kJ/mol	Joback Method
hvap	61.71	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	4.090		Crippen Method
mcvol	190.930	ml/mol	McGowan Method
pc	2412.37	kPa	Joback Method
rinpol	1737.00		NIST Webbook
tb	655.52	K	Joback Method
tc	882.93	K	Joback Method
tf	396.41	K	Joback Method
vc	0.707	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.13	J/mol×K	655.52	Joback Method
cpg	488.31	J/mol×K	693.42	Joback Method
cpg	502.36	J/mol×K	731.32	Joback Method
cpg	515.33	J/mol×K	769.22	Joback Method
cpg	527.23	J/mol×K	807.12	Joback Method
cpg	538.11	J/mol×K	845.02	Joback Method
cpg	548.00	J/mol×K	882.93	Joback Method
dvisc	0.0018085	Pa×s	396.41	Joback Method
dvisc	0.0009445	Pa×s	439.60	Joback Method

dvisc	0.0005541	Pa×s	482.78	Joback Method
dvisc	0.0003548	Pa×s	525.97	Joback Method
dvisc	0.0002431	Pa×s	569.15	Joback Method
dvisc	0.0001757	Pa×s	612.34	Joback Method
dvisc	0.0001325	Pa×s	655.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357898&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume